

# Cluster Monte Carlo Algorithm for the Quantum Rotor Model

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We propose a highly efficient “worm” like cluster Monte Carlo algorithm for the quantum rotor model in the link-current representation. We explicitly prove detailed balance for the new algorithm even in the presence of disorder. For the pure quantum rotor model with  $\mu = 0$  the new algorithm yields high precision estimates for the critical point  $K_c = 0.33305(5)$  and the correlation length exponent  $\nu = 0.670(3)$ . For the disordered case,  $\mu = \frac{1}{2} \pm \frac{1}{2}$ , we find  $\nu = 1.15(10)$ .

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What types of insulating, conducting, superconducting and more exotic phases occur in two-dimensional systems at  $T = 0$  is a topic of considerable current interest. A significant amount of theoretical [1–4] and experimental [5,6] effort has focused on bosonic systems where a superconductor to insulator transition is known to occur. In agreement with most experiments [5], it was under quite general conditions shown [1,2] that a transition can occur directly between the superconducting and insulating states. However, more recently, it has been suggested that an exotic *metallic* phase also is possible [4,6]. In this context precise numerical results would be very valuable and in the present paper we propose a new, very efficient cluster Monte Carlo algorithm for this purpose, allowing us to significantly improve previous results. In particular we show that the inequality [7]  $\nu \geq 2/d$  is *not* violated in the presence of disorder, resolving contradictions in previous work. The high precision of the algorithm should allow for precise calculations of transport properties of quantum rotor models studied theoretically in [1,4]. The ideas presented here could be useful for the study of classical spin systems [19].

Low-dimensional bosonic systems are often described in terms of the (disordered) boson Hubbard model:  $H_{\text{bH}} = \sum_{\mathbf{r}} \left( \frac{U}{2} \hat{n}_{\mathbf{r}}^2 - \mu_{\mathbf{r}} \hat{n}_{\mathbf{r}} \right) - t_0 \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} (\hat{\Phi}_{\mathbf{r}}^\dagger \hat{\Phi}_{\mathbf{r}'} + c.c.)$ . Here  $U$  is the on-site repulsion,  $t_0$  the hopping strength,  $\mu_{\mathbf{r}}$  the chemical potential varying uniformly in space between  $\mu \pm \Delta$  and  $\hat{n}_{\mathbf{r}} = \hat{\Phi}_{\mathbf{r}}^\dagger \hat{\Phi}_{\mathbf{r}}$  is the number operator. If we set  $\hat{\Phi}_{\mathbf{r}} \equiv |\hat{\Phi}_{\mathbf{r}}| e^{i\theta_{\mathbf{r}}}$  and integrate out amplitude fluctuations,  $H_{\text{bH}}$  becomes equivalent to the quantum rotor model [8]:

$$H_{\text{qr}} = \frac{U}{2} \sum_{\mathbf{r}} \left( \frac{1}{i} \frac{\partial}{\partial \theta_{\mathbf{r}}} \right)^2 + i \sum_{\mathbf{r}} \mu_{\mathbf{r}} \frac{\partial}{\partial \theta_{\mathbf{r}}} - t \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \cos(\theta_{\mathbf{r}} - \theta_{\mathbf{r}'}). \quad (1)$$

Here,  $\theta_{\mathbf{r}}$  the phase of the quantum rotor,  $t$  the renormalized hopping strength and  $\frac{1}{i} \frac{\partial}{\partial \theta_{\mathbf{r}}} \simeq n_{\mathbf{r}}$ . The quantum rotor model describes a wide range of phase transitions dominated by phase-fluctuations and it is well known [8] that an equivalent classical model exists where the Hamiltonian is written in terms of currents defined on the links

of a lattice,  $\mathbf{J} = (J^x, J^y, J^z)$ . These link-current variables describe the “relativistic” bosonic current which should be divergenceless,  $\nabla \cdot \mathbf{J} = 0$ . In terms of these variables the classical (2+1)D Hamiltonian can be written as follows [8]:

$$H = \frac{1}{K} \sum'_{(\mathbf{r}, \tau)} \left[ \frac{1}{2} \mathbf{J}_{(\mathbf{r}, \tau)}^2 - \mu_{\mathbf{r}} J_{(\mathbf{r}, \tau)}^z \right]. \quad (2)$$

$\sum'$  denotes a summation over configurations with  $\nabla \cdot \mathbf{J} = 0$ . Varying  $K$  corresponds to changing the ratio  $t/U$  in the quantum rotor model. The quantum rotor model has been extensively studied [8–10] in this representation, but a number of conclusions can be questioned due to severe finite-size effects. For notational convenience it is useful to slightly enlarge the definition of the link-currents at a given site in the following way: At each site  $(\mathbf{r}, \tau)$  in the lattice we define *six* surrounding link variables  $J_{(\mathbf{r}, \tau)}^\sigma$  where  $\sigma$  runs over  $\pm x, \pm y, \pm z$ . Note that, with this notation  $J_{(x, y, \tau)}^{-x}$  and  $J_{(x-1, y, \tau)}^x$  is the same variable, with equivalent relations in the other directions. The divergenceless constraint at the site  $(\mathbf{r}, \tau)$  can then be written:  $J^{-x} + J^{-y} + J^{-z} = J^x + J^y + J^z$ , so that the sum of the incoming and outgoing currents are equal. Conventional Monte Carlo updates [8] on this model consists of updating simultaneously four link variables. Global moves, updating a whole line of link variables thus allowing particle and winding numbers to fluctuate, are added to ensure ergodicity, but the acceptance ratio for these moves becomes exponentially small for large lattice sizes. Here we will describe a way to construct a worm-like algorithm to perform non local moves for this model.

The cluster algorithm [11–13] we propose is similar in spirit to worm algorithms [14,15] in the sense that we update the link-currents by moving a “worm” through the lattice visiting the sites  $s_i = (\mathbf{r}_i, \tau_i)$ . The links through which the worm pass are updated *during* its construction. At a given site, the links with  $\sigma$  equal to  $x, y, z$  are called outgoing links and those with  $\sigma$  equal to  $-x, -y, -z$  incoming links. When the worm is moving through the lattice the currents  $J_{s_i}^\sigma$  are updated in the following manner:

if the worm is leaving the site  $s_i$  along an outgoing link we *increment* the corresponding current:

$$J_{s_i}^\sigma \rightarrow J_{s_i}'^\sigma = J_{s_i}^\sigma + 1, \quad \sigma = x, y, \tau. \quad (3)$$

If the worm is leaving the site  $s_i$  along an incoming link we *decrement* the corresponding current:

$$J_{s_i}^\sigma \rightarrow J_{s_i}'^\sigma = J_{s_i}^\sigma - 1, \quad \sigma = -x, -y, -\tau. \quad (4)$$

The construction of the worm starts with the choice of a random initial site  $s_1 = (\mathbf{r}_1, \tau_1)$  in the space-time lattice. Then the algorithm can be decomposed in two steps. (i) The worm moves to one of the 6 neighboring sites. To decide which direction to go from a site  $s_i = (\mathbf{r}_i, \tau_i)$ , we calculate for all directions  $\sigma = \pm x, \pm y, \pm \tau$  weights,  $A_{s_i}^\sigma$ , according to local detailed balance. A good choice is:

$$A_{s_i}^\sigma = \min(1, \exp(-\Delta E_{s_i}^\sigma/K)), \quad \Delta E_{s_i}^\sigma = E_{s_i}'^\sigma - E_{s_i}^\sigma. \quad (5)$$

Here  $E_{s_i}^\sigma = \frac{1}{2}(J_{s_i}^\sigma)^2 - \mu_{\mathbf{r}_i} J_{s_i}^\sigma \delta_{\sigma, \pm \tau}$  is the contribution to the total energy from the link  $J_{s_i}^\sigma$ , before the worm moves through it.  $E_{s_i}'^\sigma$  is the energy contribution with  $J_{s_i}^\sigma$  replaced by  $J_{s_i}'^\sigma$ . By normalizing the  $A_{s_i}^\sigma$ 's we define the probabilities:  $p_{s_i}^\sigma = A_{s_i}^\sigma / N_{s_i}$ , where  $N_{s_i} = \sum_\sigma A_{s_i}^\sigma$ . A direction  $\sigma$  is then chosen according to these probabilities. (ii) Once  $\sigma$  is chosen, we update the corresponding  $J_{s_i}^\sigma$  according to the above rules, Eq. (3) and (4), and extend the worm to the new lattice site  $s_{i+1}$ . (i) and (ii) are then repeated until the worm passes through the initial site where  $s_{i+1} = s_1$ . Finally, in order to satisfy detailed balance we have to *erase* the worm with a probability determined in the following way. If  $N(\text{worm})$  and  $N(\text{no worm})$  are the normalization of the probabilities at the initial site  $s_1$  *with* and *without* the worm present, then we erase the constructed worm with a probability

$$P^e = 1 - \min(1, \frac{N(\text{no worm})}{N(\text{worm})}). \quad (6)$$

Under most conditions this probability is very small. Several points are noteworthy about this algorithm. First of all, the configurations generated during the construction of the worm are not valid ( $\nabla \cdot \mathbf{J} \neq 0$ ). However, once the construction of the worm is finished and the path of the worm closed, the divergenceless constraint is satisfied. Secondly, when the worm moves through the lattice it may pass many times through the same link and cross itself before it reaches the initial site where the construction terminates. Hence, it is crucial that the current variables are updated *during* the construction of the worm. Finally, at each step  $i$  in the construction of the worm it is likely that the worm at the site  $s_i$  will partially “erase” itself by choosing to go back to the site  $s_{i-1}$  visited immediately before, thereby “bouncing” off the site  $s_i$ .

Now we turn to the proof of detailed balance for the algorithm. Let us consider the case where the worm,  $w$ , visits the sites  $\{s_1 \dots s_N\}$  where  $s_1$  is the initial site. The

worm then goes through the corresponding link variables  $\{l_1 \dots l_N\}$ , with  $l_i$  connecting  $s_i$  and  $s_{i+1}$ . Note that  $s_N$  is the last site visited before the worm reaches  $s_1$ . Hence,  $s_N$  and  $s_1$  are connected by the link  $l_N$ . The total probability for constructing the worm  $w$  is then given by:  $P_w = P_{s_1}(1 - P_w^e) \prod_{i=1}^N A_{s_i}^\sigma / N_{s_i}$ . The index  $\sigma$  denotes the direction needed to go from  $s_i$  to  $s_{i+1}$ ,  $P_{s_1}$  is the probability for choosing site  $s_1$  as the starting point and  $P_w^e$  is the probability for erasing the worm after construction. If the worm  $w$  has been accepted we have to consider the probability for reversing the move. That is, we consider the probability for constructing an anti-worm  $\bar{w}$  annihilating the worm  $w$ . We have:  $P_{\bar{w}} = P_{\bar{s}_1}(1 - P_{\bar{w}}^e) \prod_{i=1}^N \bar{A}_{\bar{s}_i}^\sigma / \bar{N}_{\bar{s}_i}$ . Here, the index  $\sigma$  denotes the direction needed to go from  $\bar{s}_i$  to  $\bar{s}_{i+1}$ . Note that, in this case the sites are visited in the opposite order,  $\bar{s}_1 = s_1, \bar{s}_2 = s_N, \dots, \bar{s}_N = s_2$ , in general  $\bar{s}_i = s_{N-i+2}$  ( $i \neq 1$ ). Note also that,  $\bar{s}_i$  and  $\bar{s}_{i+1}$  are connected by the link  $\bar{l}_i = l_{N-i+1}$  with  $\bar{s}_N$  and  $\bar{s}_1$  connected by  $\bar{l}_N = l_1$ . With this notation we see that,  $s_i$  and  $\bar{s}_{N-i+1} \equiv s_{i+1}$  are connected by the link variable  $l_i$ . Let us now consider the case where both of the worms  $w$  and  $\bar{w}$  have reached the site  $s_i$  *different* from the starting site  $s_1$ . Since we are updating the link variables during the construction of the worm and since we are always considering moving the worm in all six directions, we have  $N_{s_i} = \bar{N}_{\bar{s}_{N-i+2}=s_i}$  ( $i \neq 1$ ). Furthermore,  $A_{s_i}^\sigma$  and  $\bar{A}_{\bar{s}_{N-i+1}=s_{i+1}}^\sigma$  only depend on the link variable  $l_i$  connecting the sites  $s_i$  and  $\bar{s}_{N-i+1}$  and we see that:  $A_{s_i}^\sigma / \bar{A}_{\bar{s}_{N-i+1}}^\sigma = \exp(-\Delta E_{s_i}^\sigma/K)$ ,  $i = 1 \dots N$ . Hence, since  $P_{s_1} = P_{\bar{s}_1}$ , we find:

$$\frac{P_w}{P_{\bar{w}}} = \frac{1 - P_w^e}{1 - P_{\bar{w}}^e} \frac{\bar{N}_{\bar{s}_1}}{N_{s_1}} \exp(-\Delta E_{\text{Tot}}/K), \quad (7)$$

where  $\Delta E_{\text{Tot}}$  is the total energy difference between a configuration with and without the worm  $w$  present. Now we consider  $P^e = 1 - \min(1, N_{s_1}(\text{no worm})/N_{s_1}(\text{worm}))$ . Here,  $N_{s_1} \equiv N_{s_1}(\text{no worm})$  is equal to  $\bar{N}_{s_1}(\text{anti-worm})$  and  $\bar{N}_{s_1}(\text{no anti-worm}) \equiv \bar{N}_{s_1}$  is equal to  $N_{s_1}(\text{worm})$ . Hence, we find for the probability to erase the worm  $P_w^e = 1 - \min(1, N_{s_1}/\bar{N}_{s_1})$  and  $P_{\bar{w}}^e = 1 - \min(1, \bar{N}_{s_1}/N_{s_1})$  for erasing the anti-worm. With this choice of  $P^e$  we satisfy detailed balance since:  $\frac{P_w}{P_{\bar{w}}} = \exp(-\Delta E_{\text{Tot}}/K)$ . Ergodicity is simply proven as the worm can perform local loops and wind around the lattice in any direction, as in the conventional algorithm.

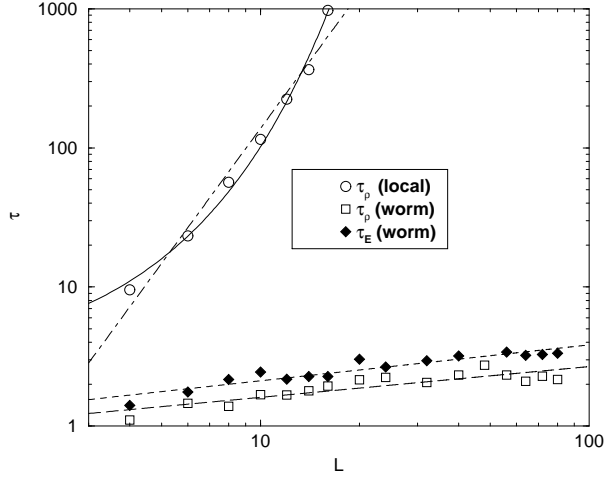


FIG. 1. Autocorrelation times versus lattice size for the conventional and worm algorithm for  $\mu = 0$  at  $K = 0.333$ . The dashed lines indicate power-law fits and the solid line an exponential fit in  $L$ .

To demonstrate the efficiency of the proposed algorithm we have calculated auto-correlation times for different lattice sizes for the worm algorithm and the conventional algorithm. For an observable  $\mathcal{O}$  we define the auto-correlation function and the auto-correlation time  $\tau_{\mathcal{O}}$  in the usual manner [16]:

$$\frac{\langle \mathcal{O}(0)\mathcal{O}(t) \rangle - \langle \mathcal{O} \rangle^2}{\langle \mathcal{O}^2 \rangle - \langle \mathcal{O} \rangle^2} = ae^{-t/\tau_1} + be^{-t/\tau_0} + \dots \quad (8)$$

Here,  $t$  is the Monte Carlo time measured in Monte Carlo sweeps (MCS), with 1 MCS corresponding to  $L^d$  attempted updates. The auto-correlation function is calculated from simulations with  $10^8$  MCS, and to obtain the best estimate of  $\tau_{\mathcal{O}}$  we always fit to the indicated double-exponential form with  $\tau_1 \ll \tau_0$ . To make a fair comparison of  $\tau_{\mathcal{O}}$  for the two algorithms, one customarily [12,16] multiplies  $\tau_{\mathcal{O}}$  for the worm algorithm by  $N/\langle l \rangle$ , with  $\langle l \rangle$  the mean number of links in a worm and  $N = 3L^3$ . With this rescaling we show in Fig. 1 the auto-correlation times,  $\tau_{\rho}$  for the stiffness (see exact definition below) at  $\mu = 0$  for both algorithms. The calculations have been performed on cubic lattices at  $K = 0.333$ , very near previous estimates of the critical point [9]. For the worm algorithm we also show the auto-correlation time for the energy,  $\tau_E$ , which is almost identical to  $\tau_{\rho}$ . The auto-correlation times increase dramatically with system size for the conventional algorithm where as they remain very small (of the order of 2-3 MCS per link) for the worm algorithm. If we fit the  $L$  dependence of  $\tau_{\rho} \sim L^{z_{MC}}$  with a power law, we obtain an auto-correlation exponent  $z_{MC}$  larger than 4 for the conventional algorithm. For the conventional algorithm it is likely that  $\tau_{\rho}$  is diverging exponentially with  $L$  since  $\rho$  is solely determined by global updates for which the acceptance probability decreases exponentially with  $L$ . For the worm algorithm we find a very small  $z_{MC} \sim 0.3$ .

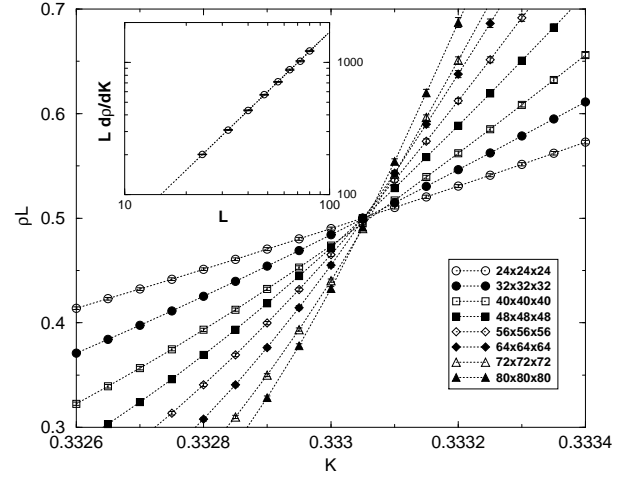


FIG. 2.  $L\rho$  versus  $K$  for different lattice sizes, for  $\mu = 0$ . All curves cross at the critical point  $K_c = 0.33305(5)$  with  $L\rho|_{K=K_c} = 0.495(5)$ . Inset:  $Ldp/dK$  at  $K_c$  versus  $L$ . The dashed line indicates a fit yielding an exponent  $\nu = 0.670(3)$ .

We now present results for the model Eq. (2) at  $\mu = 0$ . There, the model is expected to undergo a transition in the (2+1)D XY universality class [1,9] from a superfluid into a Mott insulating phase with a dynamical critical exponent  $z = 1$ . The different phases can be distinguished by calculating the stiffness defined as [8]:

$$\rho = \frac{1}{L_{\tau}L^2} \langle (\sum_{\mathbf{r},\tau} J_{(\mathbf{r},\tau)}^x)^2 \rangle. \quad (9)$$

Since we expect  $z = 1$ , we use  $L_{\tau}$ , the system size in the third direction, equal to  $L$ . To obtain the  $K$  dependence of  $\rho$  we have used reweighting techniques [17] on large runs (of the order of  $10^8$  MCS) at  $K = 0.333$ . The error bars are determined using jackknife techniques [16]. Using finite-size scaling relations, the quantity  $\rho L^z$  is expected to be independent of system size at the critical point [8],  $K_c$ . Moreover,  $L^z d\rho/dK$  is expected to diverge at  $K_c$  as  $L^{1/\nu}$  where  $\nu$  is the correlation length exponent. We have explicitly calculated this quantity by evaluating the thermodynamic derivative of  $\rho$  with respect to the coupling  $K$ :  $d\rho/dK = (\langle \rho E \rangle - \langle \rho \rangle \langle E \rangle)/K^2$ . In Fig. 2, we show  $L\rho$  versus  $K$  for different lattice sizes. From the crossing of the curves we can determine  $K_c = 0.33305(5)$  to a much higher precision than was possible using the conventional algorithm on much smaller systems [8–10]. Since all the curves cross in a single point our results are completely consistent with a dynamical exponent  $z = 1$ , as expected [1]. In the inset of Fig. 2 is shown the size dependence of  $L^z d\rho/dK$  at  $K_c$  on a log-log scale. We fit this curve to a power-law  $AL^{1/\nu}$  and obtain  $\nu = 0.670(3)$ , in perfect agreement with estimates for the three-dimensional XY universality class [18]. Preliminary results [19] for the generic transition at  $\mu = \frac{1}{4}$  show pronounced finite-size effects questioning previous work [10].

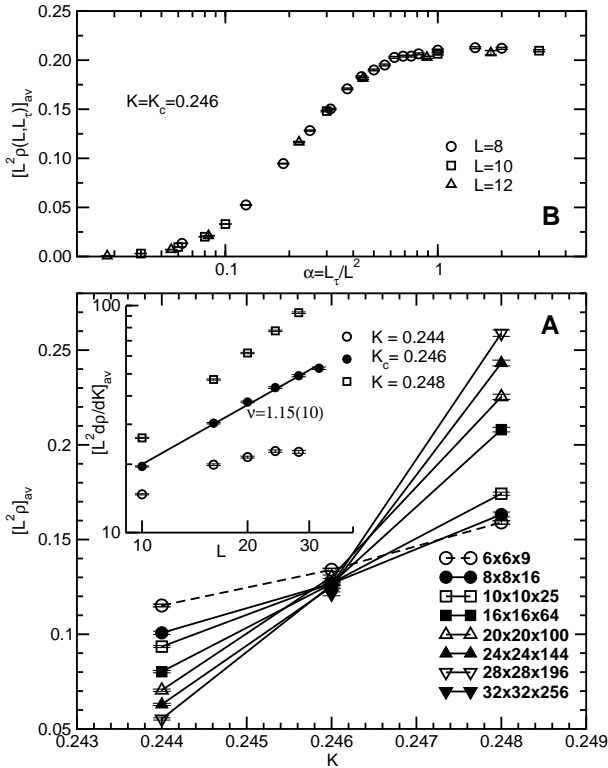


FIG. 3. (A)  $[L^2 \rho]_{\text{av}}$  versus  $K$  for different lattice sizes, for  $\mu = \frac{1}{2} \pm \frac{1}{2}$ . All curves cross at the critical point  $K_c = 0.246(1)$  with  $[L^2 \rho]_{\text{av}}|_{K=K_c} = 0.12(1)$ . Inset:  $[L^2 d\rho/dK]_{\text{av}}$  versus  $L$  for different  $K$ . The solid line indicates a power-law fit yielding an exponent  $\nu = 1.15(10)$ . (B) Scaling plot of  $L^2 \rho(L, L_\tau)$  at  $K_c = 0.246$ .

We also simulated the model Eq. (2) with disorder for  $\mu = \frac{1}{2} \pm \frac{1}{2}$ . In this case the transition is between a superfluid and an insulating boseglass phase. Scaling theory [1] predicts a second order transition with dynamical exponent  $z = 2$ . Hence, we use lattices of size  $L \times L \times \alpha L^2$  where  $\alpha = L_\tau / L^2$  is the aspect ratio. Previous work [8], limited to  $L \leq 10$ , have determined  $K_c = 0.248 \pm 0.002$ . Estimates for the correlation length exponent [8,10] yielded  $\nu = 0.9 \pm 0.1$  almost violating the inequality [7]  $\nu \geq 2/d$ . From the results shown in Fig. 3 (A), obtained with the cluster algorithm, it is clear that  $K_c$  in fact is at a slightly lower value  $K_c = 0.246(1)$ , although the crossing of  $L = 6, 8$  occurs at  $K = 0.248$ . The disorder average,  $[\cdot]_{\text{av}}$ , has been performed over 50,000 samples with  $10^5$  MCS per sample. The more precise value for  $K_c$  significantly changes estimates of  $\nu$ . The inset in Fig. 3 (A) shows  $[L^2 d\rho/dK]_{\text{av}}$  versus  $L$ , which at  $K_c$  yields  $\nu = 1.15(10)$  now largely satisfying the inequality  $\nu \geq 2/d$ . The results in Fig 3 (A) are clearly consistent with  $z = 2$ . In Fig. 3 (B) we show results for  $L^2 \rho(L, L_\tau)$  versus  $L_\tau / L^2$  at  $K_c$ . Standard scaling theory [20] predicts that this should be a universal function of  $\alpha$  if  $z = 2$ . Our results nicely confirm this. The values of exponents are in good agreement with the analytical estimates in ref. [21].

In conclusion, we have introduced a worm algorithm for the quantum rotor model. For the link-current representation of the quantum rotor model the proposed algorithm is exponentially more efficient than conventional algorithms and performs at par with the Wolff algorithm [12] for the classical 3D XY model. Most noteworthy, the algorithm performs exceptionally well on disordered systems. We have also successfully adapted it to the study of systems with longer range interactions as well as classical Ising models [19].

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